

Acetic acid, (2,4,5-trichlorophenoxy)-

Other names: (2,4,5-Trichloor-fenoxy)-azijnzuur
(2,4,5-Trichlor-phenoxy)-essigsaeure
(2,4,5-Trichlorophenoxy)acetic acid
2,4,5-T
2-(2,4,5-trichlorophenoxy)acetic acid
Acide 2,4,5-trichloro phenoxyacetique
Acido (2,4,5-tricloro-fenossi)-acetico
Arbokan
BCF-Bushkiller
Brush rhap
Brush-off 445 low volatile brush killer
Brushtox
Debroussillant concentre
Debroussillant super concentre
Decamine 4T
Ded-weed brush killer
Ded-weed lv-6 brush kil and t-5 brush kil
Envert-T
Estercide t-2 and t-245
Farmco fence rider
Fence rider
Forron
Forst U 46
Fortex
Fruitone A
Inverton 245
Kwas 2,4,5-trojchlorofenoksyoctowy
Line rider
NA 2765
Phortox
Rcra waste number U232
Reddon
Reddox
Spontox
Super D weedone
Tippon
Tippontormona
Trioxon
VEON
Veon 245

Verton 2-T

Visko rhap low volatile ester

Inchi: InChI=1S/C8H5Cl3O3/c9-4-1-6(11)7(2-5(4)10)14-3-8(12)13/h1-2H,3H2,(H,12,13)
InchiKey: SMYMJHWAQXWPDB-UHFFFAOYSA-N
Formula: C8H5Cl3O3
SMILES: O=C(O)COc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 255.48
CAS: 93-76-5

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|---------|--------------------------------------|
| gf | -306.53 | kJ/mol | Joback Method |
| hf | -450.58 | kJ/mol | Joback Method |
| hfus | 28.82 | kJ/mol | Joback Method |
| hvap | 76.65 | kJ/mol | Joback Method |
| log10ws | -2.96 | | Aqueous Solubility Prediction Method |
| logp | 3.110 | | Crippen Method |
| mcvol | 149.850 | ml/mol | McGowan Method |
| pc | 3572.80 | kPa | Joback Method |
| tb | 704.82 | K | Joback Method |
| tc | 922.43 | K | Joback Method |
| tf | 426.00 ± 2.00 | K | NIST Webbook |
| tf | 429.51 ± 0.20 | K | NIST Webbook |
| tf | 428.00 ± 0.20 | K | NIST Webbook |
| tf | 428.40 ± 0.20 | K | NIST Webbook |
| vc | 0.566 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 347.64 | J/molxK | 922.43 | Joback Method |
| cpg | 343.26 | J/molxK | 886.16 | Joback Method |
| cpg | 338.40 | J/molxK | 849.89 | Joback Method |
| cpg | 333.05 | J/molxK | 813.63 | Joback Method |
| cpg | 327.22 | J/molxK | 777.36 | Joback Method |
| cpg | 320.91 | J/molxK | 741.09 | Joback Method |

| | | | | |
|-------|-----------|---------|--------|---------------|
| cpg | 314.10 | J/molxK | 704.82 | Joback Method |
| dvisc | 0.0007091 | Paxs | 466.64 | Joback Method |
| dvisc | 0.0000544 | Paxs | 704.82 | Joback Method |
| dvisc | 0.0000735 | Paxs | 665.12 | Joback Method |
| dvisc | 0.0001030 | Paxs | 625.43 | Joback Method |
| dvisc | 0.0001513 | Paxs | 585.73 | Joback Method |
| dvisc | 0.0002349 | Paxs | 546.03 | Joback Method |
| dvisc | 0.0003908 | Paxs | 506.34 | Joback Method |
| hfust | 38.00 | kJ/mol | 428.70 | NIST Webbook |

Sources

| | |
|--|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C93765&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| Aqueous Solubility Prediction Method: | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hfust: | Enthalpy of fusion at a given temperature |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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